Atomistic simulations of carbon sputtering

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PFC meeting
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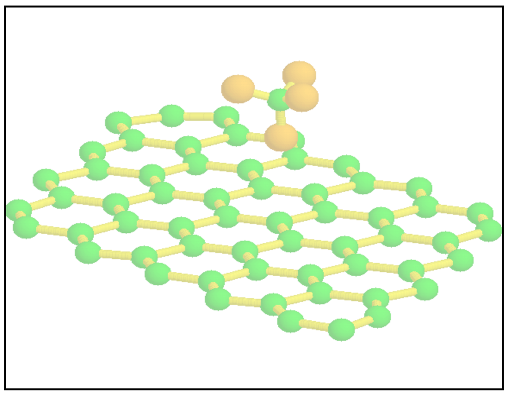

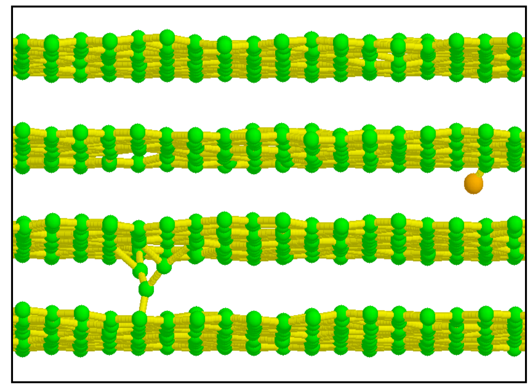

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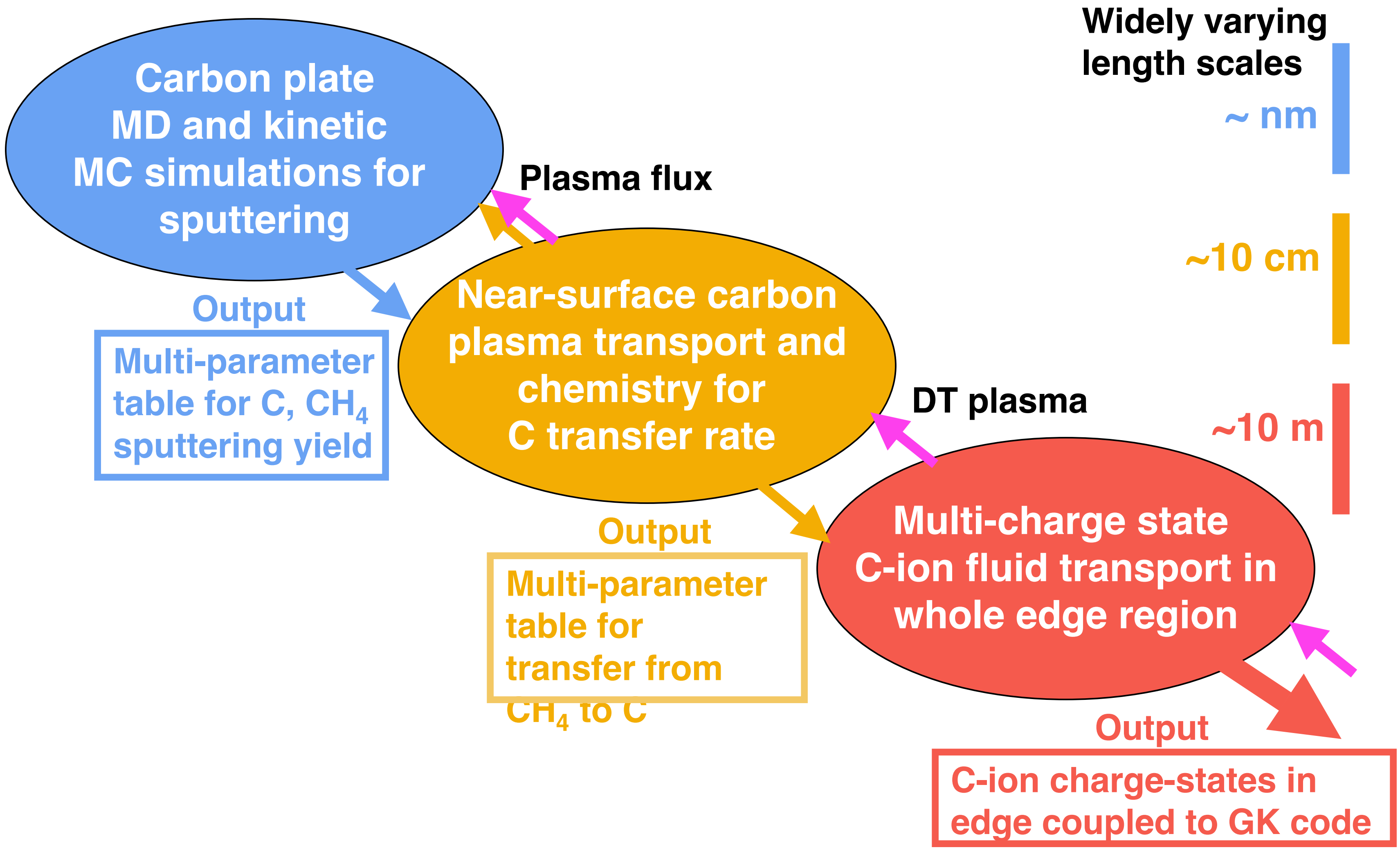
Outline

- Motivation
- LLNL work: simulations details
- Sputtering yield as a function of energy and angle
- Summary

Overall picture:
Edge plasma impurities from plasma/wall interactions

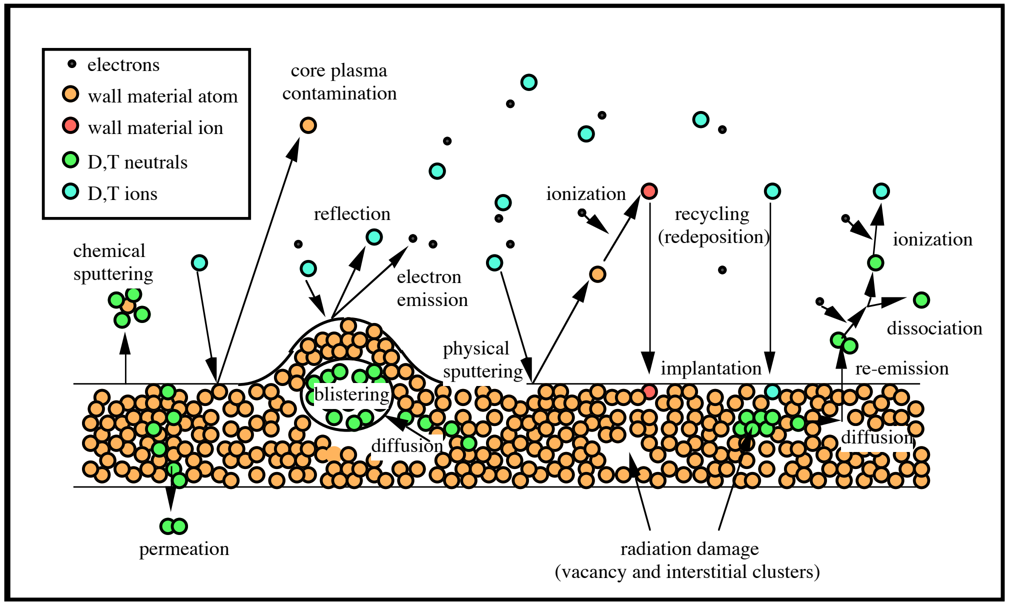
Impurities in the edge plasma are important for power balance



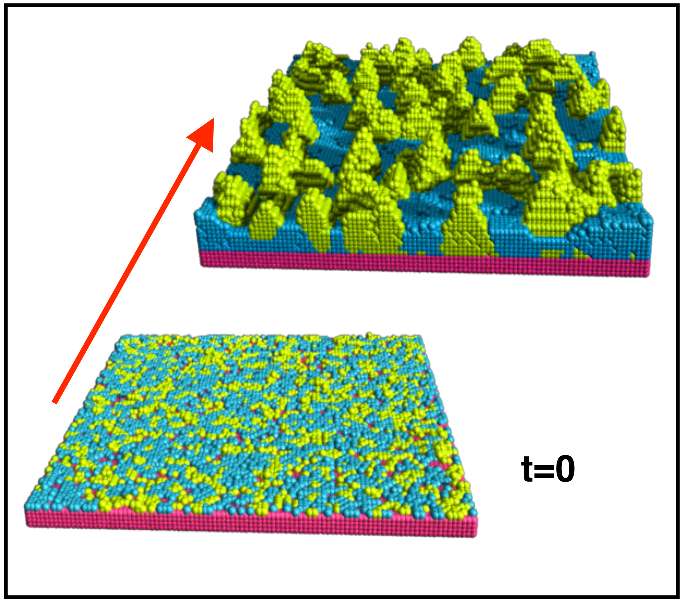
Modeling plasma-wall interactions requires understanding complex physical and chemical processes

Carbon contamination of the plasma results from erosion of the surface by chemical and physical sputtering.

Divertor surface processes



Topographical evolution



Molecular Dynamics and surface Monte Carlo simulations enable fundamental understanding and determine required sputtering-yield data

Goal: generate table of erosion as function of many variables

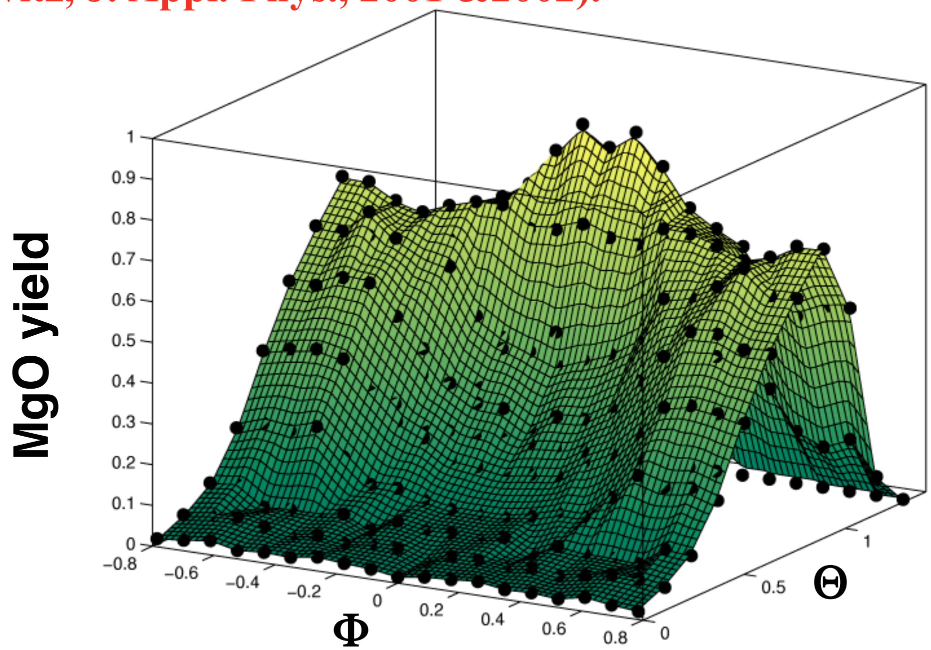
$$\text{Sputtering Yield } Y = \frac{\text{Species ejected from the surface}}{\text{Energetic ion impacting the surface}}$$

We are calculating carbon and hydrocarbon yields similar to the MgO example below (Zepeda-Ruiz & Srolovitz, J. Appl. Phys., 2001 &2002).

Yield as a function of:

- ion/neutral type
- incident energy
- incident angle
- particle flux
- surface temperature
- surface topography

Large number $O(10^5\text{-}10^6)$ of MD simulations required – use accelerated or rare event methods (future).



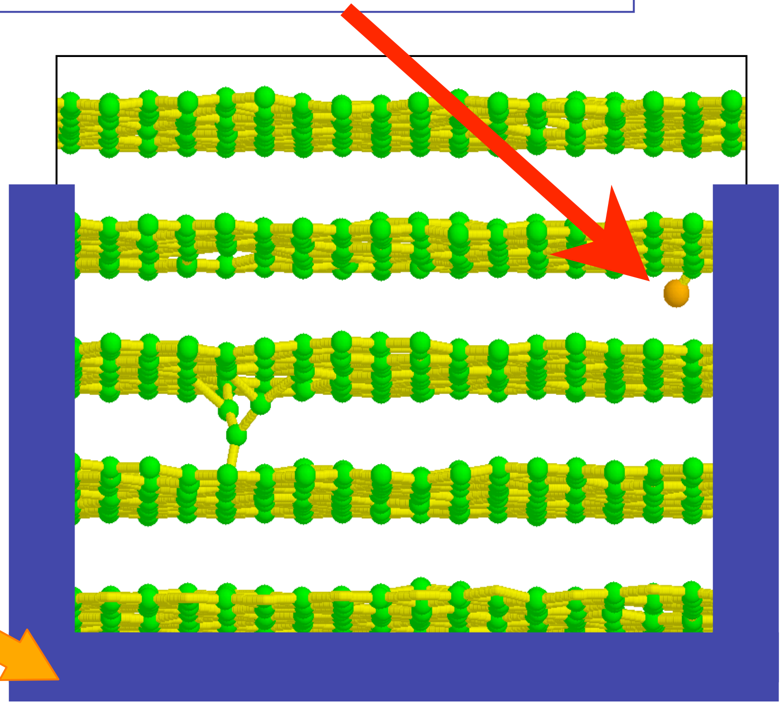
MgO sputtered by 600 eV Ar ions

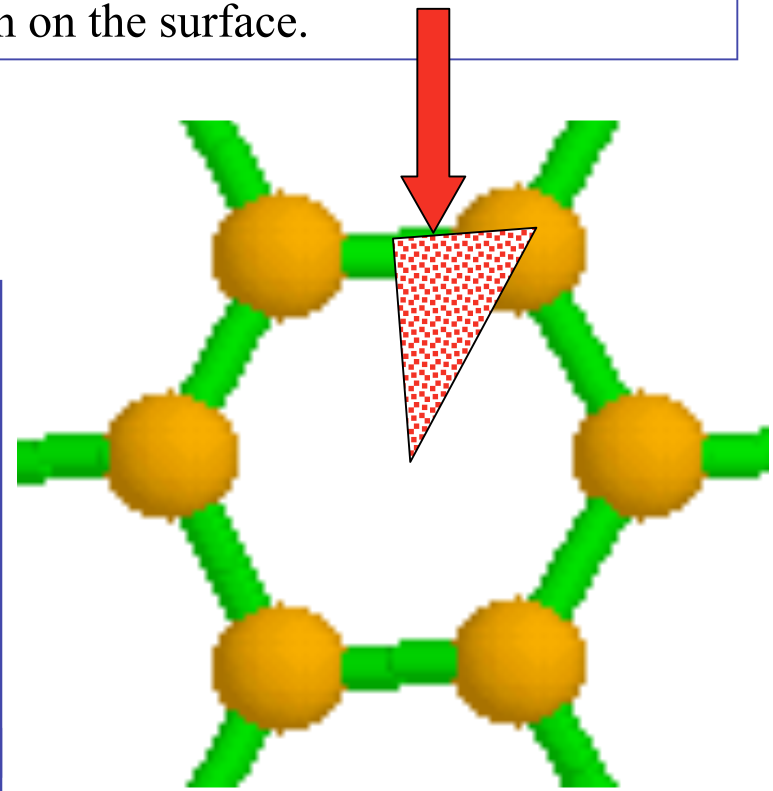
Bombardment simulations at LLNL

MDCASK (LLNL): highly parallel, variable time step, Potential: REBO+long range+ZBL
Targets: 500-40,000 C atoms, 300-600 K

H/D/T projectiles, 5-300 eV, several angles of incidence, hitting an irreducible region on the surface.

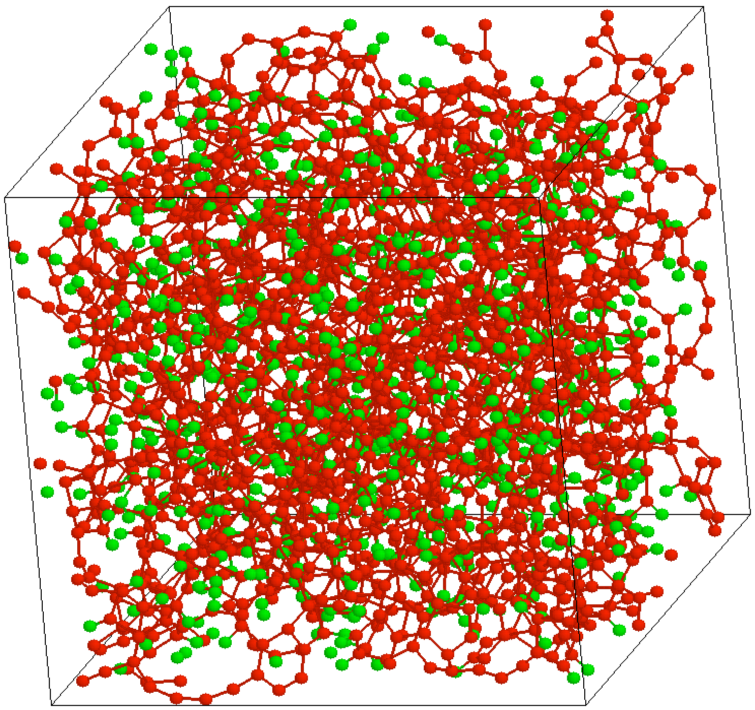
Thermostat at sides and bottom to minimize boundary effects

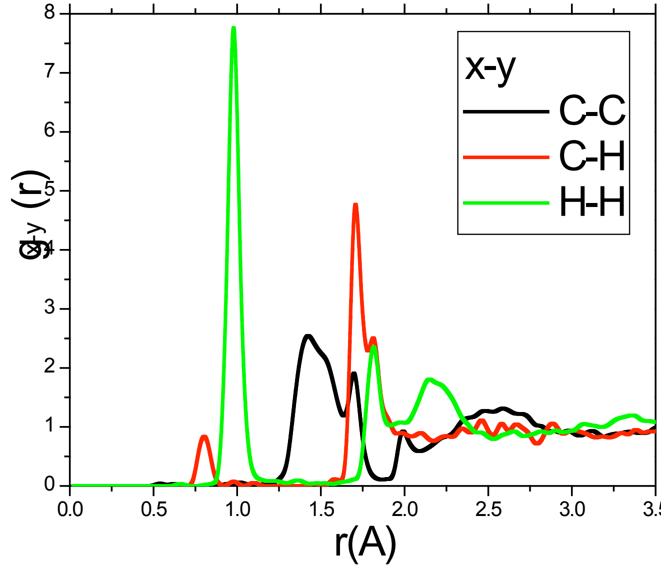




AIREBO code: original serial code (from S. Stuart) Modified to do ion bombardment.
Parallel spawning (T. Oppelstrup, LLNL) ➔
one yield point (without long range+torsion terms) takes ~1.5 hours in 20 CPU's.
(1 yield point ➔2,000 runs; 500 atoms, 0.5 ps each; i.e. ~40 ms/atom/step/CPU)

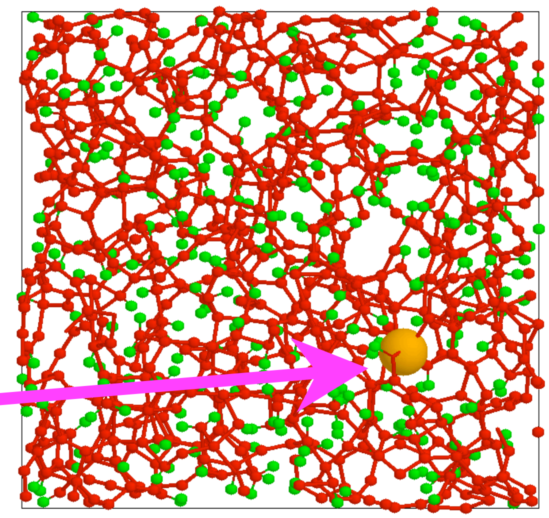
We have produced an amorphous carbon MD "sample" to model steady-state divertor surfaces with CH_x



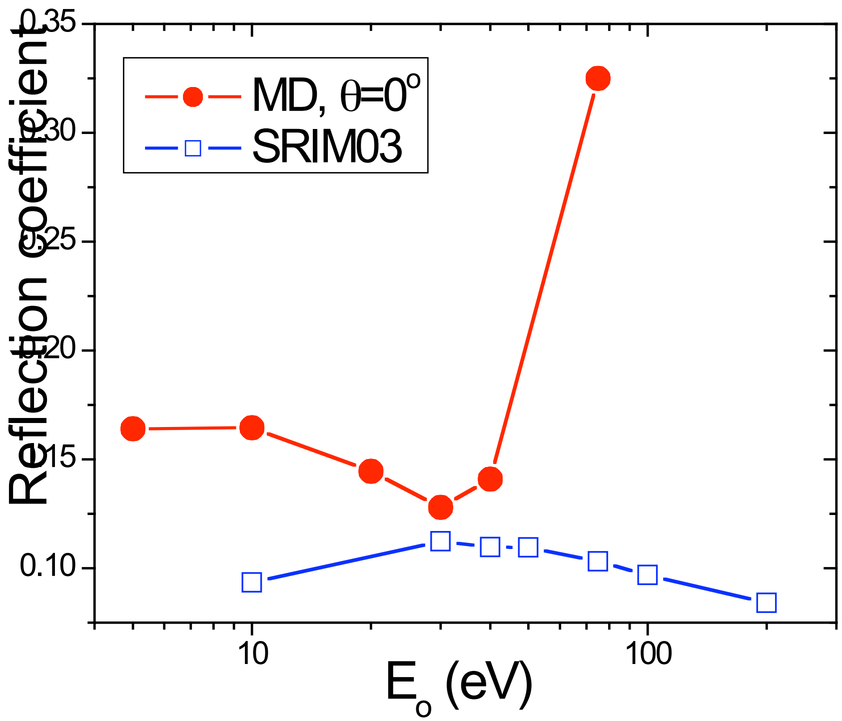


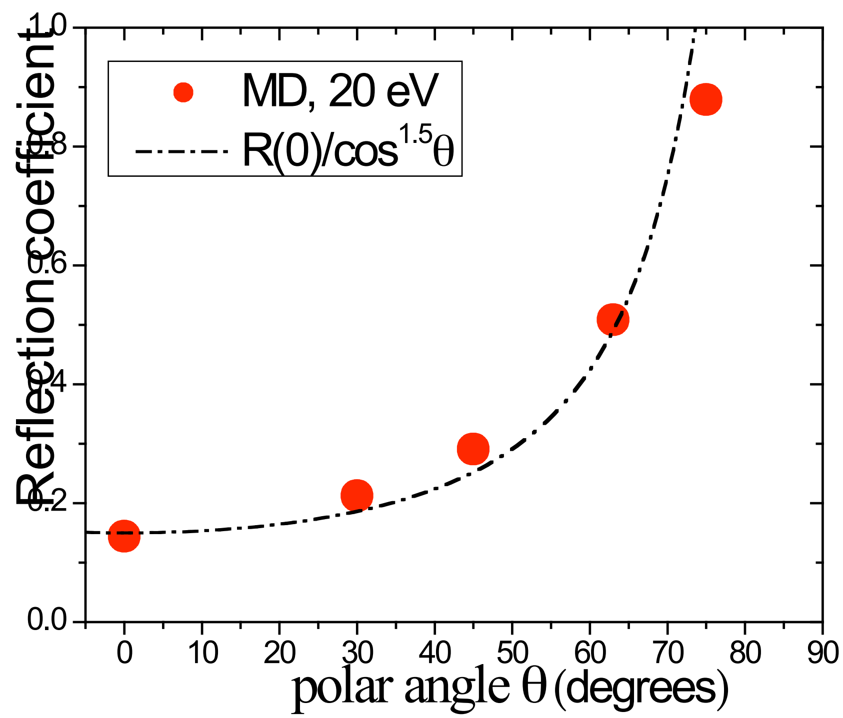
aC:H sample with 30%-40% H content
g(r) matches published results, sp^2/sp^3 ratio ~60%/40% at 300 K

100 eV D → aC:H sample, 45°, 300 K
No sputtering for this event. D gets trapped in the amorphous sample.



Calculation of reflection coefficients
T → aC:T

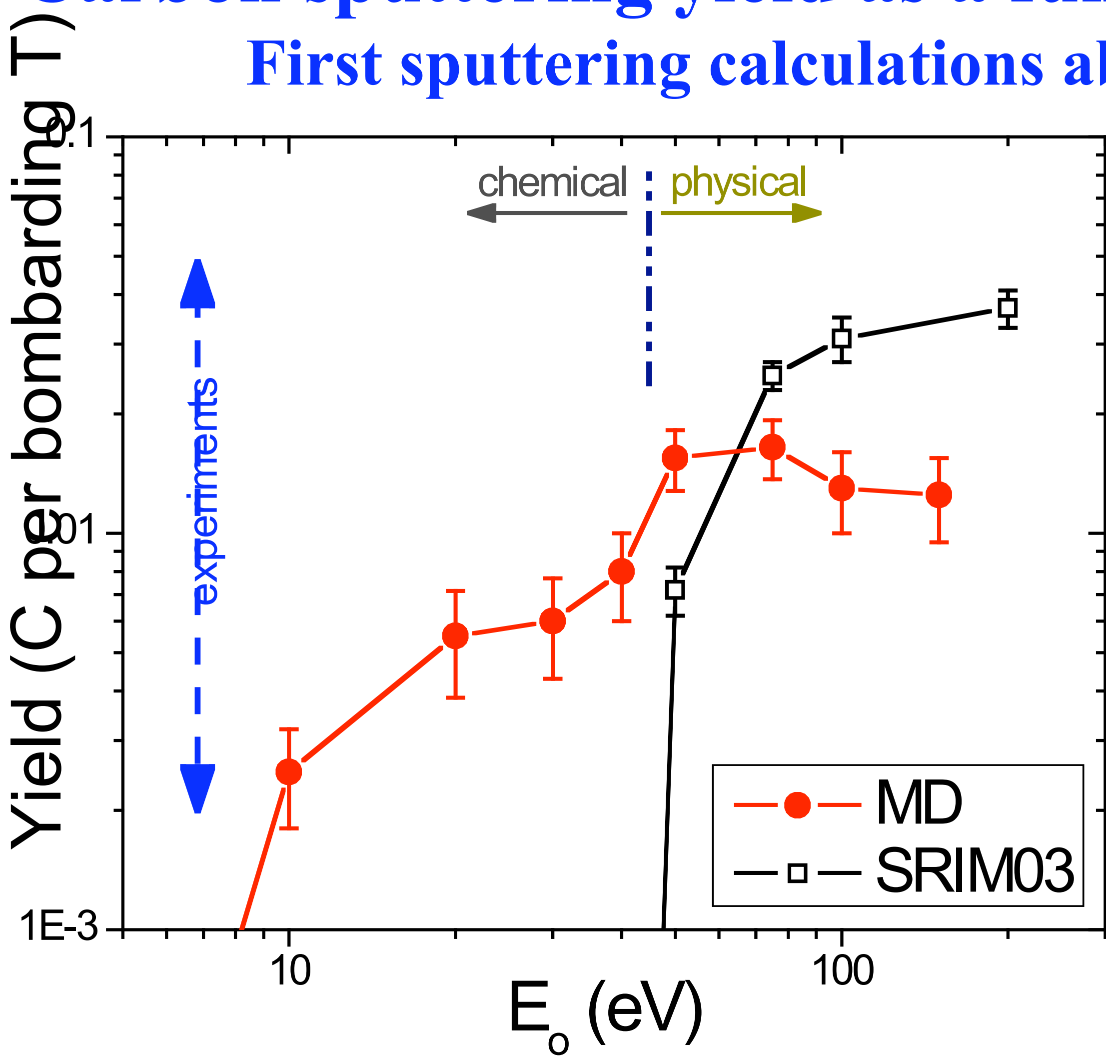




- Large differences between BCA (SRIM2003) and MD results.
- Smooth dependence with polar angle at low energies

Carbon sputtering yield as a function of energy

First sputtering calculations above 35 eV



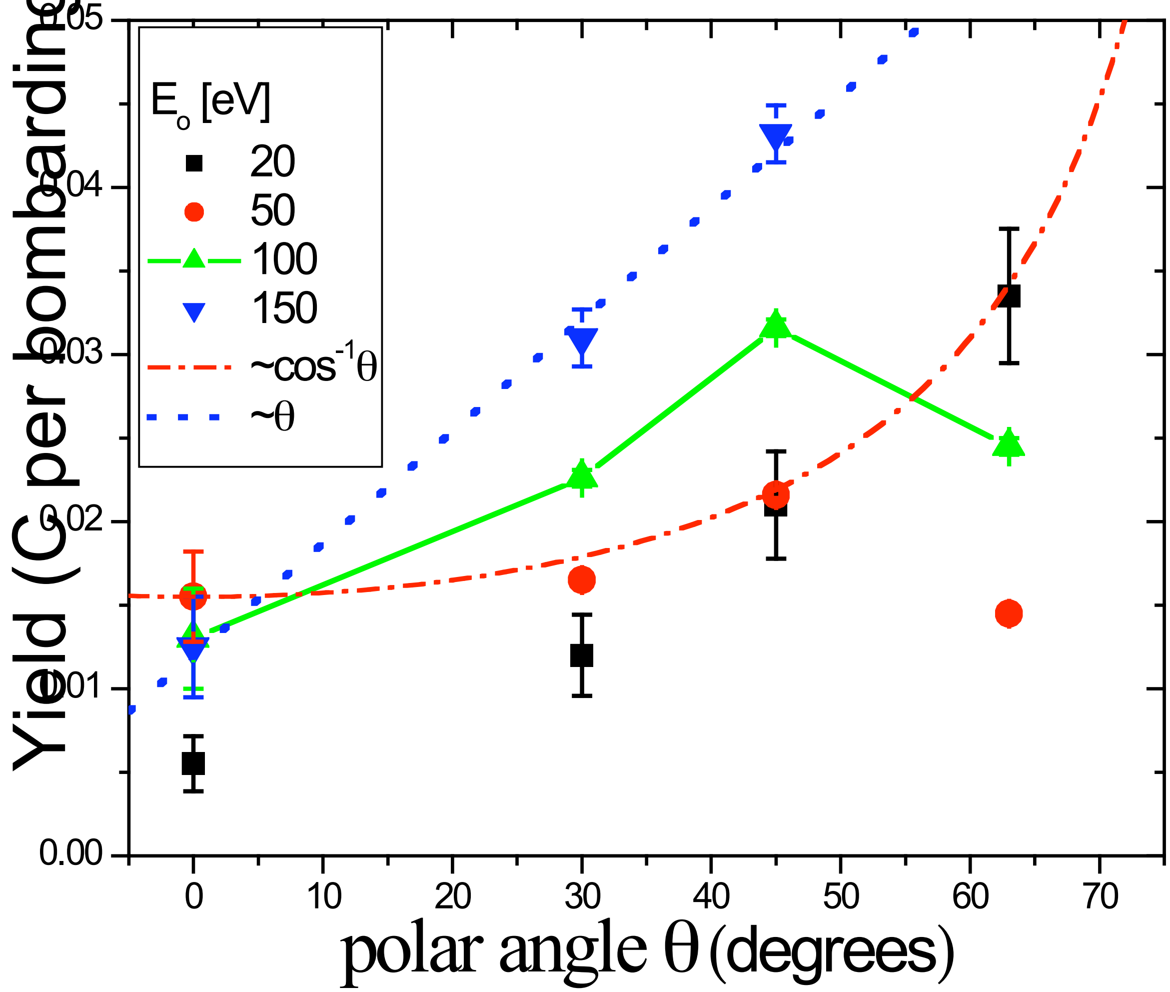
• Clear evidence of chemical erosion
• Calculated value within range of existing experimental values for H, D bombardment.

Yield is 3-8 times lower than low energy yield from Salonen *et al.*, PRB **63** (2001) 195415, for T→aC:H. Possible reasons:
• different H/C ratio (30% vs. 40%)
• Different surface topologies give different ejection probabilities.

Near future calculations:
• calculation for aC:H sample with 40% H
• to evaluate role of the surface topology, build several different surfaces and re-calculate yields

Carbon sputtering yield as a function of angle

First sputtering calculations as a function of incident angle

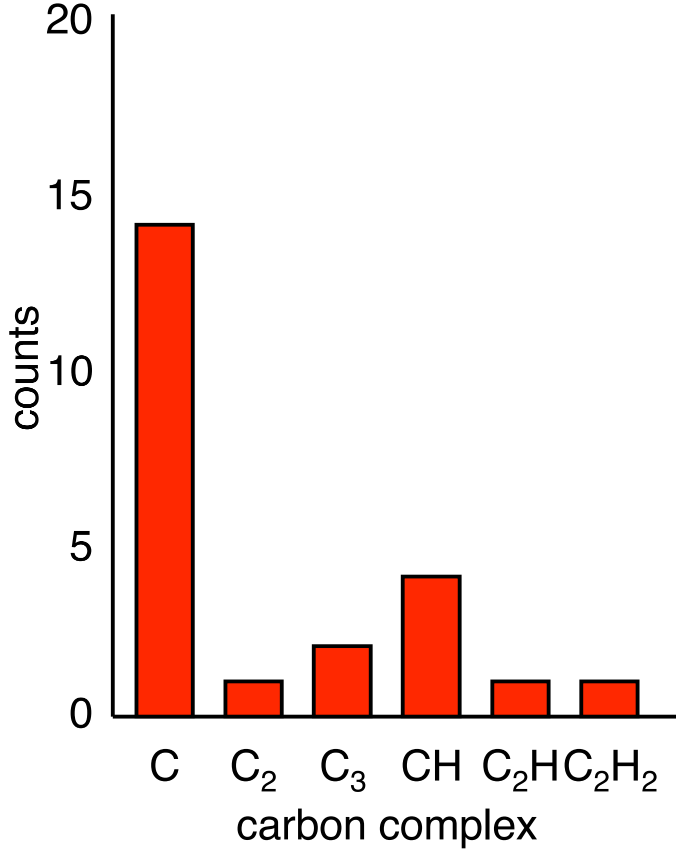


• Yield increases with the incident angle, as expected, BUT …
• There seems to be no simple functional form to fit the angular dependence.
• At high polar angles the yield decreases (very glancing incidence becomes ineffective)

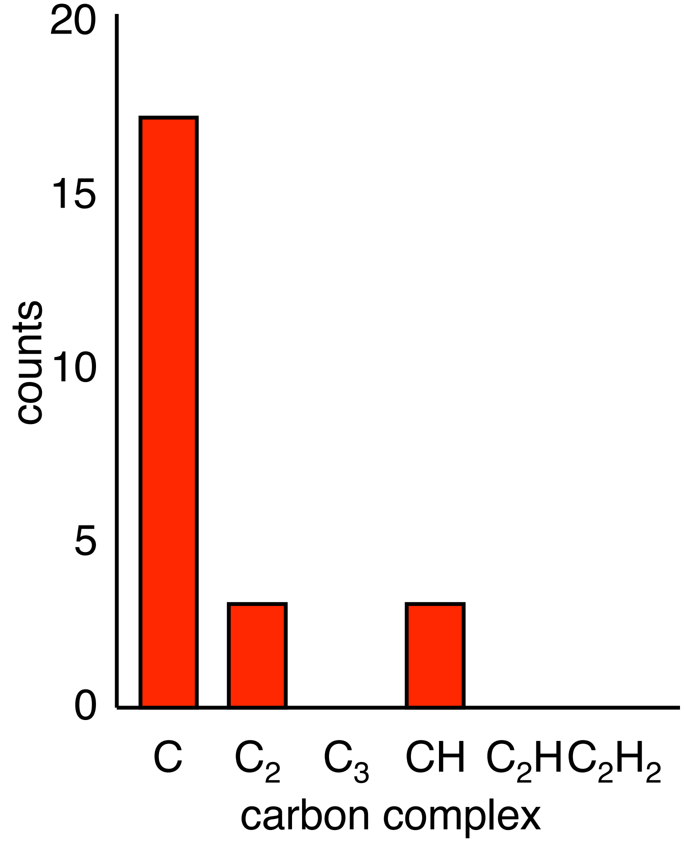
Near future calculations:
• calculation for additional angles
• to evaluate role of the surface topology, build several different surfaces and re-calculate.

Impacts produce a variety of ejected carbon complexes

case I: 50 eV at 0°, 1.55% → 31 C ejected



case II: 100 eV at 0°, 1.30% → 26 C ejected



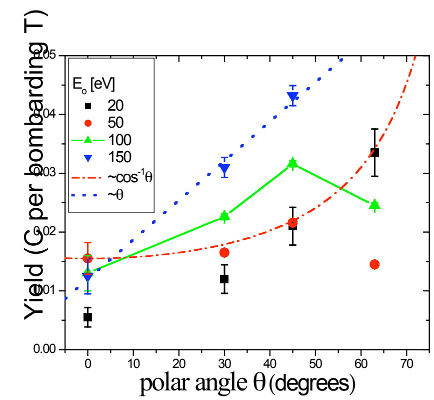
No observation of "methane" formed directly by impact/chemical sputtering

- No CH_3/CH_2 on the surface
- CT_4 could form/eject much later on, on the surface or directly above the surface → use chemical kinetics code to evaluate this possibility.

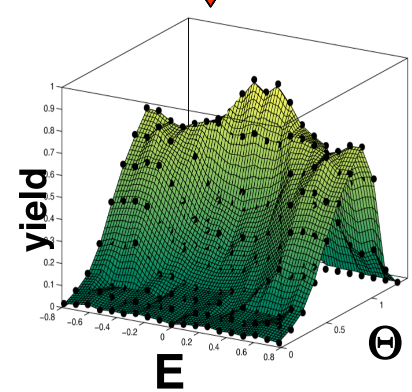
Summary and future work

CARBON SPUTTERING YIELDS:

- **MD calculations using REBO potential include both physical and chemical effects.**
- **Calculated sputtering and reflection for graphite**
- **Constructed amorphous C:H sample for MD sputtering**
- **Obtained sputtered species and erosion rates for amorphous C**



- **First sputtering calculations at energies above 35 eV**
- **First study as a function of incident polar angle**



Future calculations:

- **Sample energy and angle more finely**
- **Sample surface temperature**
- **Sample surface topology**
- **Sample target content of H/D/T**

Provide sputtering/reflection/sticking tables as input for near-surface chemistry/plasma codes